TO FIND THE ELECTRONIC AND MAGNETIC PROPERTIES OF DOUBLE PEROVSKITE La_2MMnO_6 (M=Co,Ni)

By

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Introduction/Motivation

Single & Double Perovskites

- Perovsike is calcium titanate ($CaTiO_3$) founded by Gustav Rose named given after Lev Von Perovski.
- Generally single perovskite is ABX_3 having 'A' as monovalent cation, 'B' as divalent metals cation and 'X' is a halide .
- After the complex replacement of lead in single perovskite a new structure is formed called Double Perovskites $A_2B'B''X_6$ where 'A' is a large cation and B',B'' are either trivalent or monovalent cations and 'X' is either Oxygen or Halogens[1].

[1] T. Tesfamichael, M. Roknuzzaman, C. Zhang, K. Ostrikov, A. Du, H. Wang, and L. Wang, *Scientific Reports* **9**, 718 (2019).

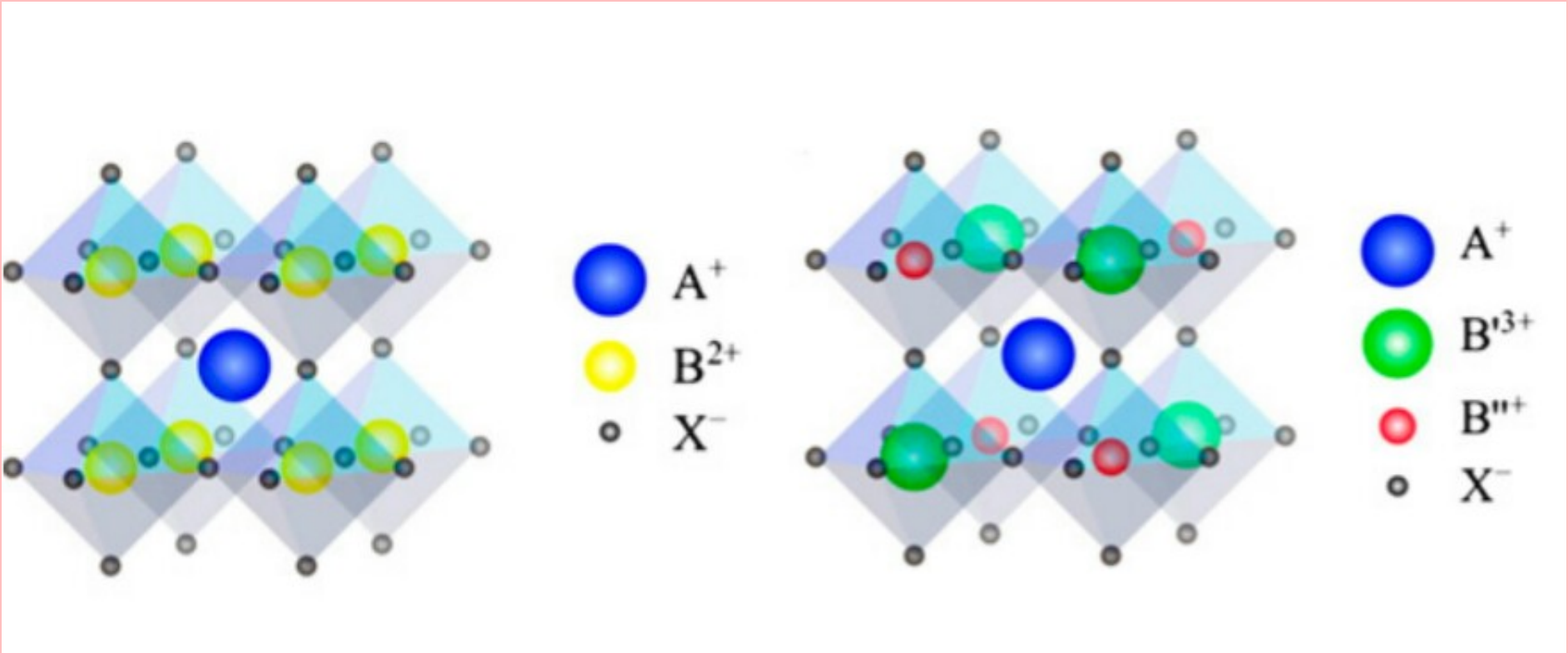

fig1:Single & Double Perovskite[2]

[2]E. L. Meyer, D. Mutukwa, N. Zingwe, and R. Taziwa, *Metals* **8,** 667 (2018).

Introduction/Motivation

Applications of Perovskites

- Applications
  - Spintronics devices
  - Light emitting diodes
  - Multistate data storage
  - In photovoltic research
- So, due to all these applications and properties it encourage me to work in this field.

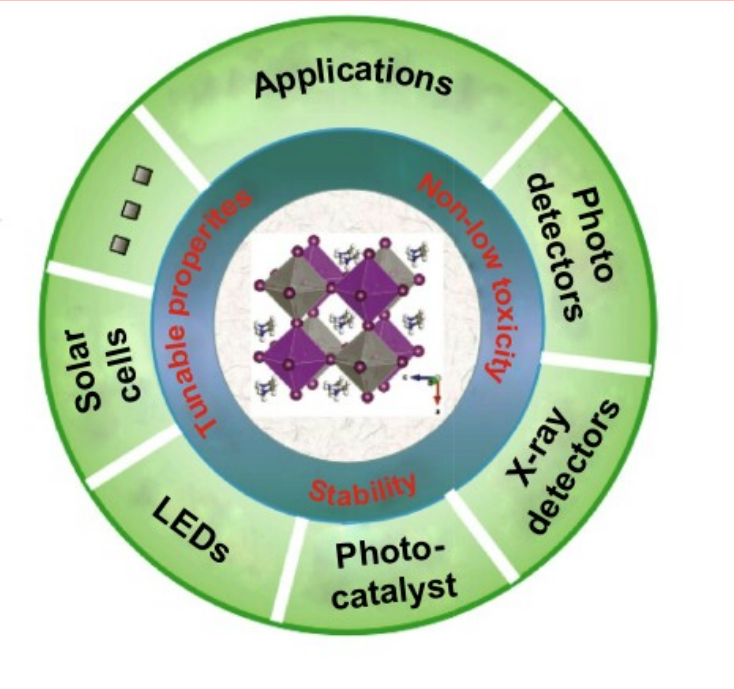

fig2:Application field of Perovskites.[a]

[a] X. Zhao *et al* *Joule* **2**, 1662 (2018).

Literature Review

- M.P Singh *et al.* (2009) studied La_2NiMnO_6, found that ordered phase has monoclinic but the disordered phase has pseudocubic structure also both can show the transition form ferromagnetic to paramagnetic[3].
- A.Kolchinskaya *et al.*(2012) studied $La_{2-x}Sr_xCoIrO_6$ and found it is antiferromagnetic also magnetic moment depends on the order of the heavy Ir ions[4].

[3] M. Singh, K. Truong, S. Jandl, and P. Fournier, *Physical Review*.**79** (2009).

[4] A. Kolchinskaya, P. Komissinskiy, M. Baghaie Yazdi, M. Vafaee Khanjani and D. Mikhailova, *et al. Physical Review*. **B 85,** 22 (2012).

Literature Review

- Z.Y Wu *et al.*(2013) observed La_2NiMnO_6 for the adsorption of bovine serum albumin protein and found that it has highest adsorbtion capacity at 850^0C it adsorb 219.6 mg/g shows that it is very useful in the biomedical[5].
- G.Kafle *et al.* (2015) studied Nd_2MgIrO_6 and found it is Antiferromagntic in ground state also it is Mott-Hubbard type insulator with space group of $P2_1/n$,Monoclinic distorted double perovskite result potential V_{Nd} =6ev , and V_{Ir} = 1.25 ev Also Nd couples antiferromagnetic with Ir[6].

[5] Z.-Y. Wu, C.B. Ma, X.G. Tang, R. Li and Q.X. Liu, *et al. Nanoscale Research Letters*. **8**, 207 (2013).

[6] M. Ghimire, G. Kaphle, and R. Thapa, *Journal of Nepal Physical Society* **3**, 50 (2016).

Literature Review

- P. Kumar *et al.* (2016) observed by doping *La* in $Sr_{(2-x)}La_xNiMoO_6$ and found that electric conductivity is high for concentration 0.04[7].
- E. Meyer *et al.*(2018) found the Goldschmith tolerance factor(t) of halide perovskite were $0.81 \leq t \leq 1.0$ which also gives the concept of lanthanide based halide double perovskite[8].

[7] P. Kumar, N. K. Singh, G. Gupta, and P. Singh, *RSC Advanced* ,**6** (2016).
[8] E. L. Meyer, D. Mutukwa, N. Zingwe, and R. Taziwa, *Metals* **8,** 667 (2018).

Objectives

- **General Objectives**
  - To identify the ground state electronic configurations of La_2MMnO_6 compound.
  - To study the structural properties of La_2MMnO_6 compound.
  - To compare the obtained result with the available experimental results.
- **Specific Objective**
  - Study of the electronic and magnetic properties of La_2MMnO_6compound.

Theoretical background and methodology

Many body Hamiltonian

$$\hat{H}\psi_i(\mathbf{R}_I, \mathbf{r}_i) = E_i\psi_i(\mathbf{R}_I, \mathbf{r}_i) \tag{1}$$

where the hamiltonian can be written as,

$$\hat{H} = \hat{T} + \hat{V} \tag{2}$$

$$\hat{H} = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + \sum_I \frac{\mathbf{P}_I^2}{2M_I} - \sum_I \frac{Z_I e^2}{|\mathbf{r} - \mathbf{R}_I|} + \frac{1}{2}\sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2}\sum_{I \neq J} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|} \tag{3}$$

- K. E. of electrons and K. E. of nuclei.
- P. E due to the attration between electron-nucleus.
- P. E due to repulsive between electron-electron .
- P. E due to repulsive between nucleus-nucleus.

Born-Oppenheimer Approximation

$$\hat{H} = \sum_i \frac{\mathbf{p}_i^2}{2m_i} - \sum_I \frac{Z_I e^2}{|\mathbf{r} - \mathbf{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{4}$$

- K. E. of nuclei (neglected) because M/m>>> 10^3 so V<<<v (molecular confirmation)
- Nucleus-nucleus replusive P. E (constant).

Hartree-Fock Approximation:

System of N electrons, the antisymmetrized wave function is given by the following slater determinant.

$$\psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{r}_1,\mathbf{s}_1) & \phi_1(\mathbf{r}_2,\mathbf{s}_2) & .. & .. & \phi_1(\mathbf{r}_N,\mathbf{s}_N) \\ \phi_2(\mathbf{r}_1\mathbf{s}_1) & \phi_2(\mathbf{r}_2,\mathbf{s}_2) & .. & .. & \phi_2(\mathbf{r}_N,\mathbf{s}_N) \\ .. & .. & .. & .. & .. \\ \phi_N(\mathbf{r}_1,\mathbf{s}_1) & \phi_N(\mathbf{r}_2,\mathbf{s}_2) & .. & .. & \phi_N(\mathbf{r}_N,\mathbf{s}_N) \end{vmatrix} \tag{5}$$

Hartree-Fock equations is given as follows:

$$\left[\sum_i \frac{\mathbf{p}_i^2}{2m} - \sum_{i=1}^{N}\sum_{I=1}^{M} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \sum_{j\neq i} \int d\mathbf{r}' \phi_j^*(\mathbf{r}') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \phi_j(\mathbf{r}')\right] \phi_i(\mathbf{r})$$

$$- \sum_{j\neq i} \left[\int d\mathbf{r}' \phi_j^*(\mathbf{r}') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \phi_i(\mathbf{r}') \delta_{\sigma_i\sigma_j}\right] \phi_j(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r}) \tag{6}$$

Density Functional Theory DFT

- The HF approximation mostly used in pre DFT era was based on Slater determinant form of single electron wave function was lengthy process and problematic too.
- The basic approach of DFT is to develop exchange and correlation energy in terms of electron density

$$n(\mathbf{r}) = N \int \int ... \int \psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)^* \psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)\, d^3 r_1\, d^3 r_2 ... d^3 r_N \tag{7}$$

Kohn-Sham equation

Kohn-Sham equation can be written as,

$$\left[-\frac{1}{2}\nabla_i^2 + V_{eff}(\mathbf{r}_i) \right] \psi_i \quad = \quad \epsilon_i \psi_i \tag{8}$$

Where V_{eff} is Effective Kohn-Sham potential

Local Density Approximation (LDA)

$$E_{xc}^{LDA}[n] = \int n(\mathbf{r})\epsilon_{xc}[n(\mathbf{r})]d\mathbf{r}. \quad (9)$$

where $\epsilon_{xc}[n(\mathbf{r})]$ is a exchange- correlation energy per particle of a uniform gas of interacting electrons of density $n(r)$.

Comptational Approach

- The mode of study will be computational which will be conducted using WEIN2K package.The WEIN2K package is a computer program which performs quantam mechanical calculations on periodic solids and it is written in Fortan.
- For some cases we will use Quantum Espresso(QE) whenever it required.

Expected Outcomes

We expect to find out the band structure of La_2MMnO_6 (M=Co,Ni) compound and some of the structural, electronic and magnetic properties of La_2MMnO_6(M=Co,Ni) compound.

Time schedule

Work	Time Duration (in Months)					
	1-2	3-4	5-6	7-8	9-10	11-12
Literature Review						
Software Familiarization						
Data Enumeration & Calculation						
Data Analysis & Paper Publishing						
Thesis Writing & Documentation						

References

1. T. Tesfamichael, M. Roknuzzaman, C. Zhang, K. Ostrikov, A. Du, H. Wang, and L. Wang, *Scientific Reports* **9**, 718 (2019).
2. E. L. Meyer, D. Mutukwa, N. Zingwe, and R. Taziwa, *Metals* **8,** 667 (2018).
3. M. Singh, K. Truong, S. Jandl, and P. Fournier, *Physical Review*.**79** (2009).
4. A. Kolchinskaya, P. Komissinskiy, M. Baghaie Yazdi, M. Vafaee Khanjani and D. Mikhailova, *et al. Physical Review*. **B 85,** 22 (2012).
5. Z.-Y. Wu, C.B. Ma, X.G. Tang, R. Li and Q.X. Liu, *et al. Nanoscale Research Letters*. **8**, 207 (2013).
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7. P. Kumar, N. K. Singh, G. Gupta, and P. Singh, *RSC Advanced* ,**6** (2016).
8. E. L. Meyer, D. Mutukwa, N. Zingwe, and R. Taziwa, *Metals* **8,** 667 (2018).

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Thank you
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